Solids

Byungjoon Min

December 5, 2018

Department of Physics, Chungbuk National University

Density of States (Free Particles)

Consider particles in a box with $V = L \times L \times L$.

$$\Psi(x, y, z) = \left(\frac{2}{L}\right)^{3/2} \sin(k_x x) \sin(k_y y) \sin(k_z z),$$

$$E_n = \frac{\hbar^2 k^2}{2m}, \quad k_x = \frac{n_x \pi}{L}, \quad k_y = \frac{n_y \pi}{L}, \quad k_z = \frac{n_z \pi}{L},$$

where n_x, n_y, and n_z are integer. Thus,

$$k^2 = \frac{\pi^2}{L^2}(n_x^2 + n_y^2 + n_z^2) = \frac{\pi^2}{L^2} r^2.$$

where $r^2 = n_x^2 + n_y^2 + n_z^2 = \left(\frac{kL}{\pi}\right)^2$.

Density of States (Free Particles)

The total number of states $G(k)$ with k-vectors of magnitude between 0 and k is one-eighth (1/8) of the volume of the sphere of radius r,

$$G(k) = \frac{1}{8} \times \frac{4}{3}\pi r^3 = \frac{1}{8} \times \frac{4}{3}\pi \left(\frac{kL}{\pi}\right)^3.$$

And, the density of states is

$$g(k)dk = \frac{dG(k)}{dk}dk = \frac{1}{8} \times 4\pi k^2 \left(\frac{L}{\pi}\right)^3 dk = \frac{Vk^2}{2\pi^2}dk.$$

Density of States (Electron)

Electrons in solids (metals) are fermions and are not fixed in number. The density of states in k-space is the same as

$$g(k)dk = \frac{Vk^2}{2\pi^2}dk.$$

For the density of state in energy space,

$$\epsilon = \frac{\hbar^2 k^2}{2m}, \quad d\epsilon = \frac{\hbar^2}{2m}(2k)dk,$$

$$\begin{aligned} g(\epsilon)d\epsilon &= 2 \times \frac{Vk^2}{2\pi^2}\frac{m}{\hbar^2 k}d\epsilon = 2 \times \frac{V}{2\pi^2}\frac{m}{\hbar^2}kd\epsilon \\ &= 2 \times \frac{V}{2\pi^2}\frac{m}{\hbar^2}\frac{\sqrt{2m\epsilon}}{\hbar}d\epsilon = \frac{mV}{\pi^2\hbar^3}\sqrt{2m\epsilon}d\epsilon, \end{aligned}$$

where 2 is for two different spins.

Fermi Energy

Boundary between occupied and unoccupied states in energy space is called the Fermi energy ϵ_F. The Fermi energy for free electron gas can be computed as

$$\begin{aligned} N &= \int_0^{\epsilon_F} \frac{mV}{\pi^2\hbar^3}\sqrt{2m\epsilon}d\epsilon \\ &= \frac{(2\epsilon_F m)^{3/2}}{3\pi^2\hbar^3}V. \end{aligned}$$

Defining $\rho = N/V$, the Fermi energy is

$$\epsilon_F = \frac{\hbar^2}{2m}(3\rho\pi^2)^{2/3}.$$

Total Thermal Energy

The total energy is then

$$
\begin{aligned}
E &= \int_0^{\epsilon_F} \epsilon g(\epsilon) d\epsilon \\
&= \int_0^{\epsilon_F} \epsilon \frac{mV}{\pi^2 \hbar^3} \sqrt{2m\epsilon} d\epsilon \\
&= \frac{mV}{\pi^2 \hbar^3} \sqrt{2m} \int_0^{\epsilon_F} \epsilon^{3/2} d\epsilon \\
&= \frac{mV}{\pi^2 \hbar^3} \sqrt{2m} \frac{2}{5} \epsilon_F^{5/2} \\
&= \frac{\hbar^2 (3\pi^2 N)^{5/3}}{10\pi^2 m} V^{-2/3},
\end{aligned}
$$

where

$$
\epsilon_F = \frac{\hbar^2}{2m} (3\rho\pi^2)^{2/3}.
$$

Degeneracy (Exclusion) Pressure

Since $dE = -PdV$,

$$dE = \frac{\hbar^2 (3\pi^2 N)^{5/3}}{10\pi^2 m} \left(-\frac{2}{3}\right) V^{-5/3} dV.$$

And the degeneracy pressure (or quantum pressure) is

$$\begin{aligned} P &= \frac{2}{3}\frac{E}{V} \\ &= \frac{2}{3}\frac{\hbar^2 (3\pi^2 N)^{5/3}}{10\pi^2 m} V^{-5/3} \\ &= \frac{\hbar^2 (3\pi^2)^{2/3}}{5m} \rho^{5/3}. \end{aligned}$$

Bloch's Theorem

Consider a periodic potential,

$$V(x+a) = V(x).$$

The solution to the Schrödinger equation for such a potential should satisfy the condition

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} + V(x)\psi = E\psi,$$
$$\psi(x+a) = e^{iKa}\psi(x).$$

Check the dirac's comb and band-gap structure.